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New helium equation of state for pressurized nanobubbles in UO2 matrix calculated via molecular dynamics simulations

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During storage helium atoms accumulate in spent fuel via alpha-decay. These helium atoms cluster into microscopic bubbles that change the physical properties of spent fuel. To estimate the impact of such bubble, it is essential to possess a good thermodynamical model for helium interacting with the surrounding matrix including states at high pressures and temperatures.
Therefore, molecular dynamics simulations are carried out to establish a new equation of state for helium in nanobubbles embedded in UO2 matrix. Four bubbles sizes, ranging from 1 to 10 nm, have been investigated for temperatures ranging from 300 to 900 K and helium concentration ranging from 3.2×10-2 to 0.39 mol/cm3. From these data, we are able to fit a new equation of state for helium using the Brearley and MacInnes'model. We observe that helium atom is heterogeneously distributed inside the nanobubble with the apparition of a boundary layer of about 1 nm thick at the surface. We also find an upper limit concentration corresponding to 1.6 helium atom per UO2 vacancy beyond which no more helium atom can be incorporated into the bubble.

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